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SECTION 11

AEROSPACE VEHICLE EXHAUST AND TOXIC CHEMICAL RELEASE

11.1 Introduction. This section of the handbook is intended to provide aerospace engineers and scientists with background information in the areas of tropospheric air quality and environmental assessment to assist them in the planning, design, testing, and operation of space vehicle systems. It deals primarily with the release of hazardous materials from the launch of space vehicle systems, spills of toxic fuels, and potential accidents.

Including the introduction, this section is organized into eight major subsections. The contents of the remaining subsections are summarized as follows:

11.1.1 TERMS. Definition of Terms Used in this Handbook:

11.1.2 Environmental Threats—Overview of the atmospheric environmental threats that may be caused by the handling, testing, and launch of space vehicle systems.

11.1.3 Meteorological Effects—Overview of the concepts of atmospheric transport and diffusion.

11.1.4 Specific Sources—Description of the specific sources of air pollutants such as rocket exhaust products, fuel spills, fires, and accidents.

11.1.5 Toxicity Criteria—Toxicity criteria for materials that have the potential of being released into the atmosphere during the handling, testing, and launch of space vehicle systems.

11.1.6 Hazard Assessment and Mitigation—Discussion of procedures for identifying and dealing with potential atmospheric environmental threats.

11.1.7 Computer Models—Discussion of computerized models that can be employed to evaluate different atmospheric hazards. Model applicability, data requirements, necessary hardware, and output are discussed.

11.2 Definitions.

ACGIH—American Council of Government and Industrial Hygienists.

AFTOX—U.S. Air Force toxic chemical dispersion model.

Al_2O_3—Aluminum oxide.

Ambient—Encompassing or surrounding.

Atmospheric Diffusion—The spreading of gaseous and/or particulate matter by turbulent motions in the atmosphere (often used interchangeably with dispersion).

Atmospheric Stability—A measure of the thermal stability or instability of the atmosphere, especially its lowest layers.

BLAST—Acoustics effects model.

BOOM—Acoustics effects model.

Ceiling—(1) Maximum short-term average concentration above which exposure should never occur. (2) Lowest height above ground level at which the clouds at and below that level obscure more than five-tenths of the total sky.

Cloud Stabilization—The point at which a cloud with initial vertical momentum and/or buoyancy ceases to rise because it has reached approximate equilibrium with ambient conditions.

Concentration—The amount (mass) of a substance in a given volume of air (as in milligrams per cubic meters) or the relative amount of a substance given as a ratio (as in parts per million).

Confidence Level—The probability that a specified concentration or dosage will not be exceeded.

Conflagration—A raging fire that results when solid fuels or propellants are ignited.

Continuous Release—A release of air pollutants over an extended period of time, as in the case of evaporation from a liquid spill or stack emissions.

CO—Carbon monoxide.

CO_2—Carbon dioxide.

Deflagration—An explosion and raging fire that occur when hypergolic liquid propellants are mixed together.

Deposition—Material deposited on the ground surface in mass per unit area (see gravitational deposition and washout).

Dispersion—The spreading of gaseous and/or particulate matter by turbulent motions in the atmosphere (often used interchangeably with diffusion).

Doppler Acoustic Sounder—A remote sensing device that uses the doppler shift of acoustic waves to measure vertical wind profiles up to a maximum of 600 to 1,000 meters above the surface.

Dosage—Time-integrated concentration (typical units are milligram minutes per cubic meter).

D2—U.S. Army chemical hazard prediction model.

D2PC—Updated version of the D2 model that is designed specifically for personal computers.

Emission Rate—Mass or quantity of an air pollutant released to the atmosphere per unit time (typical units are grams per second).

Entrain—To draw or pull into.

EPA—Environmental Protection Agency.

Evaporation Rate—Amount of vapor released to the atmosphere per unit time from the surface of a liquid (typical units are milligrams per minute).

FDH—Formaldehyde dimethylhydrazone.

Gravitational Deposition—Surface deposition (fallout) due to gravitational settling of particles or drops.

HARM—Hypergolic Accidental Release Model.

Hazard Distance—The maximum distance to a concentration, dosage, or deposition greater than or equal to a specified critical value.

HCl—Hydrogen chloride.

Hypergolic Reaction—An explosive chemical reaction that takes place when hypergolic propellants (liquid fuel and oxidizer) are mixed together.

Instantaneous Release—A short-term release of air pollutants by an explosion, flash fire, etc.

Inversion—A thermally stable atmospheric layer within which the temperature increases with increasing height.

Isopleth—A constant value line or contour level.

Lapse Rate—The rate of atmospheric temperature decrease with height.

mg/m^3—Milligrams per cubic meter.

Mixing Layer—Atmospheric layer above the surface within which vertical turbulent mixing takes place (also referred to as the mixed layer or surface mixing layer).

Mixing Layer Height—Height (depth) of surface mixing layer.

MSHA—Mine Safety and Health Administration.

NDMA—Nitrosodimethylamine.

NIOSH—National Institute of Occupational Safety and Health.

N_2H_4—Hydrazine.

NO_2—Nitrogen dioxide.

N_2O_4—Nitrogen tetroxide.

OBDG—Ocean Breeze/Dry Gulch model.

p/m or ppm—Parts per million.

Pasquill Stability Category—A letter indicator for the following six atmospheric stability categories: very unstable (A), unstable (B), slightly unstable (C), neutral (D), stable (E), and very stable (F). An extremely stable (G) category is sometimes used.

Permissable Exposure Limit (PEL)—An allowable average concentration of a pollutant, usually for an 8-hour work day.

Precipitation Scavenging—See washout.

Rawinsonde—A balloon-borne meteorological instrument package used to obtain upper-air measurements of winds, barometric pressure, temperature, and humidity.

REEDM—Rocket Exhaust Effluent Diffusion Model.

Spill Rate—Amount (mass or volume) of a chemical that escapes or spills from a casing or container per unit time.

SPILLS—A dispersion model developed by Shell Oil Company for evaporative spills.

SRB—Solid rocket booster.

SRM—Solid rocket motor.

Surface Roughness Length—A micrometeorological measure of how rough the surrounding terrain is, depending on obstacles to wind flow such as buildings, hills, trees, and vegetation.

Time-Mean Concentration—The mean concentration over a specified averaging time.

Time-Weighted Average (TWA)—See permissible exposure limit.

Troposphere—The first 10 to 17 kilometers of the atmosphere within which, on average, temperature decreases with height.

UDMH—Unsymmetrical dimethylhydrazine.

Upper-air Sounding—Vertical profiles of temperature, relative humidity, winds, and pressure versus altitude, usually obtained from rawinsonde measurements.

UTM—Universal Transverse Mercator (planetary grid system).

Vapor Pressure—The pressure of vapor in equilibrium with a liquid at a given temperature.

Washout—Surface deposition of a substance removed from the atmosphere by precipitation.

11.3 Potential Environmental Threats.

11.3.1 Overview. The handling, test firing, and launching of aerospace vehicle systems involve hazardous materials that present many potential environmental threats. Personnel, flora, fauna, equipment, and facilities are all threatened to some degree, depending on their sensitivity and the hazardous materials involved. Contact with a hazardous material may be direct (at the source) or indirect (arising from the atmospheric transport and diffusion (dispersion) of the material). In addition to hazardous materials, the launch and reentry of aerospace vehicles produce sonic booms that occasionally have adverse impacts.

The primary atmospheric environmental hazards associated with the handling, test firing, and launch of aerospace vehicle systems are produced by the fuels and propellants used by these systems. Modern space vehicle systems use both liquid and solid propellants. Although storage and handling normally do not present hazards for solid rocket motors, they do for liquid fuels. Liquid hydrogen and liquid oxygen are highly explosive, but are not otherwise a threat to the environment. Hypergolic liquid fuels, on the other hand, are extremely hazardous if released to the atmosphere by a leak or spill. The pollutants of concern in the exhaust from a liquid fueled rocket consist of both combustion products and unburned fuel and oxidizer. The unused hypergolic fuel and oxidizer in a space vehicle that returns to Earth present a hazard that should not be overlooked.

The pollutants of principal concern in current rocket exhaust clouds are aluminum oxide (Al_2O_3), hydrogen chloride (HCl), carbon monoxide (CO), hydrazine (N_2H_4), unsymmetrical dimethylhydrazine (UDMH), formaldehyde dimethylhydrazone (FDH), nitrogen tetroxide (N_2O_4), and hydrazine hydrochloride. The toxic effects of aluminum oxide are those of a nuisance dust such as irritation to the eyes and mucous membranes of the respiratory tract. Hydrogen chloride is highly corrosive to human tissue, and its inhalation can damage the teeth and irritate or damage the mucous membranes of the upper respiratory tract, depending on the concentration. Carbon monoxide has an affinity for hemoglobin 210 times that of oxygen and, by combining with hemoglobin, renders blood incapable of carrying oxygen to the tissues. Thus, carbon monoxide can cause hypoxia (oxygen deficiency), followed by unconsciousness or death at higher concentrations. Exposure to hydrazine can cause irritation of the nose and throat, followed by itching, burning, and swelling of the eyes (temporary blindness may occur) and damage the kidney, liver, and blood systems. Hydrazine also possesses carcinogenic properties. When heated, hydrazine hydrochloride decomposes into hydrazine and hydrogen chloride and may therefore have the toxic potential of both chemicals. UDMH exposure at high concentrations can lead to tremors and then seizures, and it has both mutagenic and carcinogenic properties. Because FDH breaks down into reaction products similar to those of UDMH, it is assumed to have similar toxicological properties. Nitrogen tetroxide decomposes into various nitrogen oxides of which nitrogen dioxide (NO_2) is of greatest concern. Toxic effects produced by nitrogen dioxide range from irritation of the eyes and nose to lung damage to death, depending on the exposure time and concentration.

11.3.2 Static Firings and Launches. The potential environmental threat presented by normal firings of liquid-fueled engines is small because the major pollutants in the exhaust are carbon dioxide and small amounts of nitrogen oxides and carbon monoxide. The pollutants of primary concern in the exhaust from a solid-fueled rocket motor are aluminum oxide and hydrogen chloride. Aluminum oxide, an abrasive used in many types of sanding and grinding materials, can damage optical and precision equipment. As a dust, it is subject to EPA and state ambient air quality standards for particulates with aerodynamic equivalent diameters less than 10 micrometers. However, because these standards are for long-term exposures (the standards are 24-hour average and annual geometric mean concentrations of 150 and 50 micrograms per cubic meter, respectively), the short-term impacts caused by rocket launches and test firings generally do not threaten them. Hydrogen chloride, which can exist as a vapor or in water as an acid, is both corrosive and toxic. There is some evidence that hydrogen chloride in low concentrations can adversely affect electronic equipment (ref. 11.1). In systems where deluge and/or sound suppression water is directed into the exhaust of SRM's, airborne droplets containing hydrogen chloride and other exhaust products are likely.

The degree of damage to flora by contact with a hazardous material depends on the species, the hazardous material, the magnitude of the exposure, and the ambient humidity. The presence of water on a leaf generally enhances damage. Potential threats range from partial but recoverable foliage damage to total destruction. The Air Pollution Control Association publication "Recognition of Air Pollution Injury to Vegetation: A Pictorial Atlas" (ref. 11.2), illustrates and discusses the effect on flora of many air pollutants. Experience at Kennedy Space Center (ref. 11.3) reveals that a single launch of the space shuttle can cause severe plant damage within 1 km of the launch facility, and minor loss of photosynthetic tissue due to deposition of water droplets containing aluminum oxide and hydrogen chloride has been observed more than 10 km from the launch pad. The degree of damage is spotty and varies widely with distance and from launch to launch. Over a 30-month period covering the first nine space shuttle launches, the number of plant species in the vicinity of launch complex 39A declined from an average of 7.8 per study area to 5.1. Heartier plant species have taken over the areas where other species were destroyed.

11.3.3 Accidental Releases. Many hazardous materials must be stored near rocket test or launch facilities because they are used as fuels, oxidizers, solvents, and cleaners. As indicated by the toxicity tables in section 11.6, the accidental release of any of these materials poses a serious threat to the environment. Indeed, accidental releases of hazardous materials are a far greater threat to personnel safety, flora, and fauna than are normal rocket firings. Section 11.5 provides additional information about accidental releases.

11.3.4 Acoustic Threats. The atmosphere acts as a lens that can refract acoustic (sound) waves upward or downward, depending on the vertical profile of the speed of sound. At any height in the atmosphere, the speed of sound is equal to the sum of the temperature-dependent acoustic wave propagation speed and the wind-speed component in the direction of propagation. If the speed of sound decreases with height, the acoustic wave will be refracted upward. Conversely, if the speed of sound increases with height, the acoustic wave will be refracted downward. Because the acoustic wave propagation speed increases with height in a temperature inversion (an atmospheric layer within which temperature increases with height), an inversion layer above an acoustic source (explosion, rocket firing, etc.) will cause a portion of the wave front to be refracted back to the surface with a resulting sound enhancement, especially downwind of the source. The noise produced by the firing of a space vehicle system generally does not present an environmental threat other than startling animals or triggering the fall of loose plaster on buildings in the vicinity. The launch and reentry of space vehicles usually produce sonic booms. Depending on the meteorological conditions, these booms may be focused to yield large overpressures capable of causing damage such as broken windows. The magnitude of a sonic boom, which depends on the flying vehicle's speed and size, is measured in decibels, pascals, kilograms per square meter (kg/m^2), or pounds per square foot (lb/ft^2) of overpressure. The sonic booms from conventional aircraft typically cause overpressures of 2.44

to 9.76 kg/m^2 (0.5 to 2.0 lb/ft^2), while those from the space shuttle have been as high as 29.3 kg/m^2 (6.0 lb/ft^2).

11.4 Atmospheric Effects on Transport and Diffusion. Some of the most serious environmental threats associated with the handling, test firing, and launching of space vehicle systems occur when hazardous materials are transported by the atmosphere to long downwind distances. Atmospheric conditions govern the speed and direction of downwind travel of the airborne material, the rate of dilution, and the rate of evaporation. A brief discussion of the phenomena that control atmospheric transport and diffusion processes is given below. A more detailed discussion can be found in references such as the "Handbook of Applied Meteorology" (ref. 11.4) and "Atmospheric Science and Power Production" (ref. 11.5).

Wind direction determines the direction of travel for material released into the atmosphere, and wind speed determines the time required for material to travel from the point of release to a downwind point of concern, which is often called a receptor. Wind directions are reported as directions from which the wind is blowing. For example, a north wind will transport material to the south. Calm or light and variable winds present very difficult cases because the travel path of released material is unpredictable. Consequently, precautions must be taken in all directions.

The atmospheric diffusion of a cloud or plume of gases or aerosols (small drops or particles) released near the surface is determined by atmospheric turbulence (wind fluctuations caused by atmospheric eddies) and the depth of the surface mixing layer. Wind fluctuations caused by eddies smaller than the cloud or plume mix it with ambient air, while larger wind fluctuations move the cloud or plume in its entirety. Turbulence consists of mechanical and convective components. The mechanical component is produced by forced airflow over surface roughness elements, which include vegetation, terrain, and manmade structures. Mechanical turbulence increases as the wind speed or roughness of the surface increases. Convective turbulence is caused by the eddies that occur as a result of thermal instability. The atmosphere is thermally unstable if the adiabatic (no exchange of heat with the surroundings) cooling of a small "parcel" of air displaced upward results in a parcel that is warmer (less dense) than the surrounding air. Because the parcel will then continue to rise, thermal instability acts to increase vertical motions. On the other hand, if the atmospheric temperature decreases with height less rapidly than the adiabatic rate, an air parcel adiabatically displaced upward will be colder (denser) than the surrounding air. In this case of thermal stability, buoyancy forces will act to suppress the vertical motion and return the parcel to its original level. The neutral case occurs when the atmospheric temperature decreases with height at the adiabatic rate of 0.01 °C per meter. In general, the convective component is the dominant component of atmospheric turbulence on days when winds are light and solar heating of the surface results in thermal instability, while the mechanical component is dominant at night or whenever there is an adiabatic thermal stratification. Because lower atmospheric turbulence is produced by surface effects (flow over surface roughness and surface heating), atmospheric turbulence extends through only a finite depth of the lower atmosphere. This layer in which turbulent mixing occurs is called the surface mixing layer.

Diffusion models use turbulence (wind fluctuation) measurements or stability parameters to characterize diffusion rates. The standard deviations of the wind direction and elevation angles are the most common turbulence measurements. Some stability parameters vary continuously and others divide diffusion rates into discrete categories. One of the simplest and most widely used stability classification techniques is a modified version of the scheme proposed by Pasquill (ref. 11.6). The six or seven Pasquill stability categories range from A for very unstable conditions to F or G for very or extremely stable conditions. The popularity of the Pasquill stability categories is in part explained by the fact that they can be determined from standard airport surface weather observations of wind speed, cloud cover, and ceiling height. Wind speed is used as an indicator of the mechanical component of atmospheric turbulence, while the cloud cover and ceiling height are used to modify the solar radiation incident at the top of the atmosphere. This modified solar radiation is used as an indicator of the convective component of turbulence.

Precipitation falling through an atmosphere containing a hazardous gas or aerosol tends to scavenge it and deposit it at the surface. The amount of material scavenged depends on the type and rate of precipitation and the material being scavenged. Some pollutants such as hydrogen chloride are readily absorbed by water, while others such as particulate matter depend on impaction as the removal process. Small particles may also act as nuclei for the formation of clouds and precipitation. Although precipitation scavenging can significantly reduce atmospheric concentrations of the scavenged material, the amount of material deposited at the surface can also be dramatic because material is removed from the entire vertical column through which the precipitation is falling.

Evaporative spills of hazardous liquids used as rocket propellants or for other purposes, such as cleaning solvents, are among the most serious potential environmental threats. The evaporation rate is controlled by the liquid's physical characteristics such as molecular weight and vapor pressure and meteorological factors such as the temperature and wind speed. In general, evaporation increases as the wind speed and/or temperature increase. Also, evaporative losses to the atmosphere increase as the evaporating surface area increases.

11.5 Specific Sources of Air Pollutants.

11.5.1 Storage. The major threat to the environment from a stored toxic liquid such as a hypergolic fuel or oxidizer is that a leak, spill, or handling accident may release the material into the atmosphere. In addition to the obvious threat presented by the storage of toxic fuels and oxidizers, the toxicity of other chemicals such as cleaning solvents and payload materials must be considered. Hypergolic materials (nitrogen tetroxide in particular) evaporate at ambient temperatures, producing vapors that are transported downwind and dispersed by normal atmospheric processes. Not only are hypergolic materials toxic to most life, they are highly flammable and some are corrosive. The probability of an accidental release of toxic materials from a storage facility is highest when material transfers take place. Potential release scenarios include broken transfer lines, connection failures, accidents by vehicles transporting hazardous materials, and damage to the storage facility resulting from a vehicle accident.

11.5.2 Static Firings and Launches. The exhaust products of rocket motor firings may contain hazardous materials, depending upon the chemical mix of the fuel. In general, the exhaust from rocket engines that exclusively burn liquid oxygen and liquid hydrogen or RP-1 contain water and carbon dioxide, which are not considered hazardous. All other fuels produce materials that have effects on the environment ranging from a nuisance to an extreme hazard. The current SRM’s produce exhaust clouds containing aluminum oxide, hydrogen chloride, carbon dioxide, water, nitrogen, and various other trace materials after the rapid chemical reactions have been completed. Of these materials, hydrogen chloride and aluminum oxide are hazardous. Some SRM’s contain other metals such as beryllium, which is very toxic and requires special precautions if released into the atmosphere.

Water is often injected into the exhaust of SRM's to protect the launch pad or test facility or to suppress sound. Much of this water is atomized by the mechanical shears and turbulence generated by the exhaust flows. If large quantities are used, water may be expelled onto the area near the launch pad or mixed with the exhaust gas. Droplets carried aloft with the exhaust plume may rain out of the exhaust cloud as it travels downwind, as is the case of the space shuttle (ref. 11.7). Significant quantities of hydrogen chloride and aluminum oxide can be scavenged from the exhaust cloud by this process. Water droplets which come in contact with the exhaust gases, whether from rain or dewfall prior to the launch or from the launch pad ground system, mix with the exhaust gases and leave small pools and drops of dilute hydrochloric acid on the ground in the vicinity of the launch pad. This acid is initially 2 normal, but as the water evaporates it increases to approximately 11 normal where it remains until the drop is completely evaporated. At this point, the hydrogen chloride evaporates along with the water. As the deposited acid solution evaporates, the ambient concentration of gaseous hydrogen chloride rises to a peak and then decreases as the drops are depleted, and only the acid in the surface soil and the more slowly evaporating pools are available to fuel the ambient concentration. The peak ambient hydrogen chloride concentrations measured at Kennedy Space Center after the launches of space shuttle missions 41D and 51A were 3 and 9 ppm, respectively. These peak concentrations occurred 1.5 to 2 hours after the launches. Although the ambient hydrogen chloride concentration after both missions gradually decreased to about 1 ppm within several more hours, small rises in ambient concentration were reported after sunrise for 2 days after mission 51A.

In addition to a normal firing, exhaust products can be released into the atmosphere by the accidental breakup of a SRM and the subsequent burning of its pieces on the ground, which is called a conflagration. Although the exhaust products are nearly identical to those of a normal firing, changes in the heat produced and the time elapsed while burning can cause both the magnitude of the hazard and the downwind hazard distance to be greatly increased.

As noted above, liquid-fueled rocket engines other than those fueled with liquid oxygen and hydrogen or RP-1 produce exhaust clouds that contain hazardous materials. The current hypergolic-fueled rocket engines primarily burn hydrazine-based fuels with nitrogen tetroxide as the oxidizer. The exhaust products from a normal firing of these engines include nitrogen oxides that can be toxic. A greater threat than a conflagration for these vehicles is a deflagration in which the fuel and oxidizer come in contact with each other, resulting in a hypergolic explosion. The hypergolic explosion is a fairly common event that usually takes place when a space vehicle is aborted in flight. However, there also have been cases that occurred on or near the Earth's surface. For example, a Titan II missile was involved in a hypergolic explosion near Demascus, Arkansas in 1980. More recently, a Titan 34D mission was aborted shortly after launch from Vandenberg Air Force Base, California. Hypergolic explosions produce clouds that contain nitrogen tetroxide, hydrazine, and other hazardous products. In the case of the Titan 34D event, fragments of burning solid propellant fell to the ground and produced ground fires with toxic plumes, and the hypergolic fuels of the upper stages combined to produce a toxic cloud in the lower atmosphere. Long downwind hazard distances can result from deflagrations of hypergolic-fueled space vehicle systems because of the quantities and toxicities of the materials that are released.

11.5.3 Fires. Fires that involve toxic propellants or other hazardous materials are another potential threat to the environment. In general, air pollutants released by these fires include both uncombusted toxic materials and toxic products of combustion. Because the heat generated by a fire usually is small compared to that produced by a rocket launch, the buoyant rise of the plume from a fire is generally less than that of an exhaust cloud. Consequently, fires can produce toxic clouds relatively close to the Earth's surface, resulting in little chance for dispersion to take place before the toxic clouds mix to the surface. The hazards produced by fires are very difficult to evaluate because it is difficult to quantify the amount of material involved, the efficiency of combustion, the chemical reactions that take place, and the effects of fire fighting on the combustion chemistry. Most of what is known about these fires comes from test burns of toxic materials under controlled conditions.

11.5.4 Transportation. The transportation of toxic materials presents threats to the environment resulting from numerous scenarios that are beyond the scope of the current discussion. These scenarios range from small leaks to the rupture of rail cars containing toxic materials. The U.S. Department of Transportation and most State and local governments have established rules, guidelines, and procedures for the transportation of toxic materials. These rules and procedures are established by material classification and, in some cases, by individual materials.

11.5.5 Payloads. The upper stages and the payloads of some space vehicle systems contain hazardous materials. The contents of these stages must therefore be investigated as part of the hazards analysis for the system. In addition to fuels and oxidizers, electrical and other power sources may contain hazardous materials. Also, nuclear power sources are common for some types of payloads. Although the threat of radioactive hazards goes beyond the scope of this document, it is mentioned here for completeness.

11.6 Toxicity Criteria. The chemical formulas, molecular weights, and chemical abstract service (CAS) numbers for air pollutants that are contained in rocket exhaust clouds or that may be released by spills of liquid rocket fuels are listed in tables 11-1 and 11-2, respectively. Table 11-2 also includes other hazardous liquids such as cleaning solvents that are commonly found at test and launch facilities. The exposure criteria that have been established for the toxic pollutants in tables 11-1 and 11-2 by the Occupational Safety and Health Administration (OSHA), the Mine Safety and Health Administration (MSHA), the National Institute of Occupational Safety and Health (NIOSH), and the American Council of Government and Industrial Hygienists (ACGIH) are summarized in tables 11-3 and 11-4. The exposure criteria used by the U.S. Air Force and implemented in its AFTOX dispersion model for fuel spills (ref. 11.8) are listed in table 11-5. There are two types of exposure criteria. The first, a permissible exposure limit (PEL) or time-weighted average (TWA), usually represents an allowable average concentration for an 11-hour work day. The second is a ceiling or maximum short-term average concentration above which exposure should never occur. In 1989, OSHA promulgated PEL's and ceilings and proposed new values to take effect in 1992 (Ref. 11.9). Both sets of exposure criteria are listed in tables 11-3 and 11-4. In addition to the toxicity criteria in tables 11-3 and 11-4, there may also be state, local, or other criteria applicable to a specific facility. For space shuttle firings, the Committee on Toxicology (ref. 11.10) recommends 1-hour and 24-hour short-term public exposure emergency guidance levels of 1 ppm of HCl.

TABLE 11-1. Chemical Formulas, Molecular Weights, and Chemical Abstract Service Numbers for Rocket Exhaust Products.

CHEMICAL	CHEMICAL FORMULA	MOLECULAR WEIGHT	CAS NO.
Aluminum Oxide	Al_2O_3	101.96	1344–28–1
Hydrogen Chloride	HCl	36.46	7647–01–0
Carbon Monoxide	CO	28.01	630–08–0
Hydrazine	N_2H_4	32.06	302–01–2
Unsymmetrical (1,1–) Dimethylhydrazine (UDMH)	$(CH_3)_2N_2H_2$	60.12	57–14–7
Formaldehyde Dimethylhydrazone (FDH)	$(CH_3)_2N{-}N{=}CH_2$	72.11	2035–89–4
Nitrogen Tetrozide	N_2O_4	92.02	10544–72–6
Hydrazine Hydrochloride	$N_2H_4 \cdot HCl$	68.52	2644–70–4

TABLE 11-2. Chemical Formulas, Molecular Weights, and CAS Numbers for Liquid Rocket Fuels, Solvents, and Cleaners.

CHEMICAL	CHEMICAL FORMULA	MOLECULAR WEIGHT	CAS NO.
Aerozine–50	$(CH_3)_2N_2H_2 \cdot N_2H_4$	41.81	8065–75–6
Hydrazine	N_2H_4	32.06	302–01–2
Hydrazine (54%)	$N_2H_4 \cdot H_2O$	50.07	7803–57–8
Unsymmetrical (1,1–) Dimethylhydrazine (UDMH)	$(CH_3)_2N_2H_2$	60.12	57–14–7
Monomethylhydrazine (MMH)	$CH_3N_2H_3$	46.09	60–34–4
Fuming Nitric Acid (IRFNA)	HNO_3	57.20	7697–37–2
Nitrogen Tetroxide	N_2O_4	92.02	10544–72–6
n-Butyl Alchohol	$CH_3(CH_2)_3OH$	74.12	71–36–3
t-Butyl Alchohol	$(CH_3)_3COH$	74.12	75–65–0
Benzene	C_6H_6	78.12	71–43–2
Freon 12	Cl_2CF_2	120.91	75–71–8
Isopropyl Ether	$(CH_3)_2CHOCH(CH_3)_2$	102.18	108–20–3
Acetone	CH_3COCH_3	58.08	67–64–1
Xylene	C_8H_{10}	106.17	1330–20–7

Table 11-3. Exposure criteria for rocket exhaust products.

Chemical	OSHA[a]			MSHA[b]		NIOSH[b]		ACGIH[b]	
		PEL	Ceiling	TWA	Ceiling	TWA	Ceiling	TWA	Ceiling
Aluminum Oxide	1989: 1992:	15(10)mg/m³[c] 10(5)mg/m³[c]	— —	—	—	—	—	—	—
Hydrochloric Acid	1989: 1992:	— —	5.0 p/m* 5.0 p/m	—	5.0 p/m	—	—	—	—
Carbon Monoxide	1989: 1992:	50 p/m 35 p/m	— 200 p/m	50 p/m	—	35 p/m (10-h)	200 p/m	50 p/m	400 p/m (15-min)
Hydrazine	1989: 1992:	1.0 p/m 0.1 p/m	— —	1.0 p/m	—	—	0.04 mg/m³ (2-h)	0.1 p/m	—
Unsymmetrical (1,1-) Dimethylhydrazine (UDMH)	1989: 1992:	0.5 p/m 0.5 p/m	— —	0.5 p/m	—	—	0.15 mg/m³ (2-h)	0.5 p/m	—
Formaldehyde Dimethylhydrazone (FDH)	1989: 1992:	0.5 p/m 0.5 p/m	— —	0.5 p/m	—	—	0.15 mg/m³ (2-h)	0.5 p.m	—
Nirogen Tetroxide	1989: 1992:	— —	5.0 p/m[d] 1.0 p/m[d] (15-min)	—	5.0 p/m[d]	—	1.0 p/m[d] (15-min)	3.0 p/m[d]	—
Hydrazine Hydrochloride	1989: 1992:	— —	— —	—	—	—	0.04 mg/m³ (2-h)	—	—

a. PEL is 8-h average and ceiling is maximum instantaneous concentration unless otherwise specified.
b. TWA is 8-h average and ceiling is maximum instantaneous concentration unless otherwise specified.
c. Total dust (respirable dust).
d. Exposure criteria are for NO_2; molecular weight for NO_2 of 46.01 should be used to convert hydrazine concentrations to p/m for comparison with exposure criteria.
* p/m = parts per million.

Table 11-4. Exposure criteria for liquid rocket fuels.

Chemical		OSHA[a]		MSHA[b]		NIOSH[b]		ACGIH[b]	
		PEL	Ceiling	TWA	Ceiling	TWA	Ceiling	TWA	Ceiling
Aerozine–50		—	—	—	—	—	—	—	—
Hydrazine	1989: 1992:	1.0 p/m* 0.1 p/m	— —	1.0 p/m		—	0.04 mg/m³ (2-h)	0.1 p/m	—
Hyrazine (54%)	1989: 1992:	1.0 p/m 0.1 p/m	— —	1.0 p/m	—	—	0.04 mg/m³ (2-h)	0.1 p/m	—
Unsymmetrical (1,1-) Dimethylhydrazine (UDMH)	1989: 1992:	0.5 p/m 0.5 p/m	— —	0.5 p/m	—	—	0.15 mg/m³ (2-h)	0.5 p/m	—
Monomethylhydrazine (MMH)	1989: 1992:	— —	0.2 p/m 0.2 p/m	—	0.2 p.m	—	0.08 mg/m³ (2-h)	—	0.2 p/m
Fuming Nitric Acid (IRFNA)	1989: 1992:	2.0 p/m 2.0 p/m	— —	2.0 p/m	—	2.0 p/m (10-h)	—	—	—
Nitrogen Tetroxide	1989: 1992:	— —	5.0 p/m[c] 1.0 p/m[c] (15-min)	—	5.0 p/m[c]	—	1.0 p/m[c] (15-min)	3.0 p/m[c]	—
n-Butyl Alcohol	1989: 1992:	100 p/m —	— 50 p/m	100 p/m	—	—	—	—	50 p/m
t-Butyl Alcohol	1989: 1992:	100 p/m 100 p/m	— —	100 p/m	—	—	—	100 p/m	
Benzene	1989: 1992:	— —	— —	—	25 p/m	0.1 p/m (10-h)	1.0 p/m (15-min)	10 p/m	—
Freon 12	1989: 1992:	1,000 p/m 1,000 p/m	— —	1,000 p/m	—	—	—	—	—

Table 11-4. Exposure criteria for liquid rocket fuels (continued).

Chemical	OSHA[a]		MSHA[b]		NIOSH[b]		ACGIH[b]	
	PEL	Ceiling	TWA	Ceiling	TWA	Ceiling	TWA	Ceiling
Isopropyl Ether	1989: 500 p/m 1992: 500 p/m	— —	250 p/m	—	—	—	250 p/m	—
Acetone	1989: 1,000 p/m 1992: 750 p/m	— —	1,000 p/m	—	590 mg/m³ (10-h)	—	750 p/m	—
Xylene	1989: 100 p/m 1992: 100 p/m	—	—	—	100 p/m (10-h)	200 p/m (10-min)	—	—

a. PEL is 8-h average and ceiling is maximum instantaneous concentration unless otherwise specified.
b. TWA is 8-h average and ceiling is maximum instantaneous concentration unless otherwise specified.
c. Exposure criteria are for NO_2; molecular weight for NO_2 should be used to convert hydrazine concentrations to p/m for comparison with exposure criteria.
* p/m = parts per million.

TABLE 11-5. U.S. Air Force Exposure Criteria For Rocket Exhaust Products And Liquid Rocket Fuels.

CHEMICAL	TWA[a]
Hydrogen Chloride	3.0 p/m
Carbon Monoxide	100 p/m
Nitrogen Tetroxide	2.0 p/m
Aerozine-50	0.03 p/m
Hydrazine (54%)	0.02 p/m
Fuming Nitric Acid (IRFNA)	2.0 p/m
n-Butyl Alcohol	50 p/m
t-Butyl Alcohol	100 p/m
Benzene	10 p/m
Freon-12	100 p/m
Isopropyl Ether	250 p/m
Acetone	1,000 p/m
Xylene	100 p/m

a. TWA is 8-h average.
p/m = parts per million

11.7 Standard Hazard Assessment and Mitigation Procedures.

11.7.1 General. Standard assessment and mitigation procedures for the potential atmospheric hazards associated with the handling, test firing, and launching of space vehicle systems typically consist of identification and quantification of the threats, preparation of operations and contingency plans, training, and implementation. At most installations, a team under the direction of the safety office or similar organization is in place to perform these tasks. Each activity or process that could release a hazardous material to the atmosphere should be identified in advance (see section 11.3 for a discussion of the most common threats and section 11.5 for additional details). Mathematical simulation models such as those described in section 11.8 can then be used to quantify the magnitude of each potential hazard. Based on the results of this quantitative hazard assessment, operations and contingency plans should be developed to minimize each potential hazard. For example, transfer operations for toxic liquids can be restricted to periods when meteorological conditions are such that an accidental release would be unlikely to produce hazardous concentrations in downwind areas where access cannot be restricted. Operations and contingency plans with clearly defined responsibilities must be developed, and employees must be trained in their required actions under both routine and emergency conditions. All employees should know and be trained to perform their responsibilities in the event of a planned or accidental release long before the release occurs. It is highly desirable to test operations and contingency plans in simulated routine and emergency scenarios to refine and improve these plans as well as to train employees.

Preplanning for possible events that may threaten the environment is a management responsibility, but management must be provided with sufficient information to make informed decisions when developing routine operational procedures, contingency plans, and emergency response procedures such as evacuation and decontamination procedures. The availability of the necessary resources under adverse conditions must be addressed as part of the planning process. For example, if computer facilities are required, arrangements must be made for backups in the event of a power failure. Similarly, provision must be made for communications in the event of a power outage that would render most telecommunication systems unusable. Also, if predictive models are used in hazard assessment during routine or emergency operations, the data required to execute these models must be routinely acquired and available for use.

11.7.2 Storage. A procedure should be established to maintain a current inventory of all materials located at each installation where space vehicle activities take place. This inventory should include the materials, amounts, locations, possible hazards, toxicity levels, and any special emergency procedures to be followed. Liquid hydrogen, liquid oxygen, and hypergolic materials require special storage facilities. Housekeeping and inspection programs must be ongoing because neglect and corrosion are likely causes of leaking containers. Evaporative losses to the atmosphere increase as the evaporating surface area increases. Consequently, containment is generally required to retain any spilled material within a specific area and prevent the development of a large evaporating surface. Many storage facilities include a means of covering the containment area to prevent evaporation into the atmosphere. The possibility of vandalism must be considered at every storage site. Preventive measures such as security, restricted access, and shielding may be required. Proper controls and accurate inventories must be maintained for all hazardous materials. Employees at storage sites must be trained in all aspects of hazardous material storage and handling. Plans for a material transfer and the necessary precautions must be completed well in advance of the actual transfer. All potential release scenarios should be considered, and responses to these scenarios such as decontamination and/or cleanup should be part of employee training. Employees must be kept in a ready state and must be thoroughly familiar with their responsibilities in order to prevent breakdowns and confusion in the event of an accident.

11.7.3 Static Firings and Launches. The static firing of a rocket engine or motor or the launch of an aerospace vehicle system produces a large, thermally buoyant cloud of exhaust products that usually includes toxic materials. This cloud grows rapidly through the entrainment of ambient air and rises until it reaches approximate equilibrium with the surrounding atmosphere. Because this exhaust cloud cannot be prevented, a static firing or launch must be planned and conducted so as to minimize its downwind impact. This mitigation is typically accomplished by restricting static firings and launches to periods when atmospheric conditions are not conducive to pollutant concentration, dosage, or deposition values that may have an unacceptable impact in uncontrolled areas. Atmospheric transport and diffusion (dispersion) models normally are used to define the atmospheric constraints on a static firing or launch and may be used in near real time to assist in operational go/no-go decisions. In addition to considering normal firings and launches, model calculations should be performed for all credible accident scenarios (i.e., conflagrations and deflagrations). Sound propagation models can be used in a similar manner to minimize adverse noise impacts.

11.7.4 Mathematical Modeling. Mathematical models such as those described below in section 11.8 often play a key role in hazard assessment and mitigation procedures. If so, procedures for the routine execution of the selected models must be established and followed. Also, the individuals responsible for performing the model calculations must have a working knowledge of the concepts upon which they are based as well as be entirely familiar with their operational details. If a model is only executed on occasion or the person performing the model calculations is not qualified, erroneous predictions, breakdowns, and confusion can be expected, especially under the pressure of an emergency. As indicated above, all required model inputs must be readily available on a timely basis.

It is important that the output of mathematical models used for hazard assessment meet the requirements of the end user, typically the safety office, program manager, or other decision makers. Thus, several different output formats such as overlays and tabular listings may be required. Because the units of the model output should be clearly understood by the end user, provisions should always be made for conversion between metric and English units.

As an example of a typical procedure for using a hazard assessment model, assume that a dispersion model is routinely used at the launch complex for a hypergolic-fueled space vehicle. The meteorological parameters required as input to the model are routinely measured and also forecasted. At the start of each day, the planned operations are reviewed and the model is executed for all possible release scenarios for the toxic propellants under existing or forecast meteorological conditions. The model's predictions are then presented in an appropriate format to the safety office or other users, and the predictions are also filed for future reference. The model predictions are updated as required throughout the day's operations to reflect changes in meteorological or other conditions. In the event that a release to the atmosphere occurs, a post-event analysis is performed to determine the model's performance through a comparison of model predictions with all available measurements.

11.7.5 Briefings. The manner in which a mathematical model's predictions are presented to management and others is as important as the accuracy of the predictions themselves. During the planning stages, management and other users should be provided with a detailed explanation of the selected models, and they should participate in the development of formats for briefing materials that best meet their needs. If a selected model is designed to be safe-sided (i.e., biased toward overestimation of potential hazards), as is the case with most hazard assessment models, decision makers should be made aware of this fact. The information presented to decision makers should avoid superfluous details in order to avoid confusion. Graphical presentations, such as the depiction of the predicted hazard area on an installation map, can be a very effective means of providing readily understandable results. However, too much graphical detail (for example, concentration isopleths well below the hazard criterion that cover large areas) can be misleading and should be avoided. In general, a briefing should not go beyond describing the magnitude and area of the potential hazard in the user's terms. If there is no predicted hazard, a simple statement to that effect is usually all that is needed.

11.7.6 Public Awareness. Contingency plans for planned or accidental releases of toxic materials to the atmosphere must recognize the possibility that these materials could be transported to uncontrolled areas in hazardous concentrations. The elected and appointed public officials responsible for these uncontrolled areas should be briefed on the potential hazards and the actions that have and will be taken to prevent or minimize adverse impacts. Written agreements between the test or launch facility and external agencies such as fire and police departments should be negotiated to define areas of responsibility and actions to be taken in the event of a planned or accidental release. To the extent possible, external agencies should be encouraged to participate in the routine training exercises in order to test the contingency plans. If it is anticipated that planned test or launch activities will require temporary restricted access to or evacuation of some normally uncontrolled areas, the general public as well as their officials should be made aware of these requirements and the reasons why they are necessary. Press releases to the local news media and public meetings are some techniques used to inform the public of plans to protect their safety.

11.8 Computer Models.

11.8.1 Background. Table 11-6 summarizes the computerized models most frequently used in quantitative hazard assessments for rocket motor or engine test firings, space vehicle launches, and related activities that could release hazardous materials to the atmosphere. The computer resources required by these models are summarized in table 11-7. With the exception of the BLAST and BOOM sound propagation models, all of the models in table 11-6 are atmospheric transport and diffusion (dispersion) models. (In addition to the dispersion models in table 11-6, a products of combustion atmospheric dispersion (PCAD) model is currently being privately developed.) Although all of the dispersion models in table 11-6 except the empirical OB/DG model are based on widely used Gaussian diffusion model concepts, there are significant differences in model complexity and the applications for which they are designed. An overview of each model is given below with greatest emphasis placed on the rocket exhaust effluent diffusion model (REEDM) because it is the only model applicable to static firings, normal launches, conflagrations, and deflagrations. REEDM was originally developed under the sponsorship of the NASA George C. Marshall Space Flight Center (MSFC), Space Science Laboratory (ref. 11.11) to provide near real-time predictions of rocket exhaust concentrations in support of space shuttle missions. The NASA/MSFC multilayer diffusion model (ref. 11.12) was used to test and develop the procedures and algorithms used within REEDM (refs. 11.13–11.15) before the model was used to support the first launches of the space shuttle from Kennedy Space Center. REEDM has been and is undergoing continuous improvement under the sponsorship of the U.S. Air Force and NASA for use at Kennedy Space Center and Vandenberg Air Force Base. Requests for information pertaining to this diffusion model technology should be directed to the Environmental Analysis Branch, Earth Sciences and Application Division, Space Science Laboratory at NASA Marshall Space Flight Center.

11.8.2 REEDM Version 7. The REEDM version 7 computer program (ref. 11.16) is used to assess the air quality impacts of the exhaust products produced by large rocket motors or the burning of rocket fuels. The model is designed to calculate peak and time-mean concentration, dosage, and surface deposition (resulting from both gravitational settling and precipitation scavenging) of exhaust cloud constituents downwind of normal launches, launch failures, and static firings. There are several modes which this model can be used: normal launch mode in which everything operates normally, conflagration mode where an on pad explosion ruptures the SRB's casings, and finally the deflagration mode which simulates a catastrophic fireball caused by a hypergolic liquid reaction.

REEDM also incorporates three modes of operation: operational, research, and diagnostic. The operational mode is designed for launch-support operations and automatically calculates many necessary program input variables. The research mode permits the user to examine and change program parameters (e.g., fuel loads, diffusion parameters, etc.). In the diagnostic mode, a very detailed output of the model calculations may be obtained.

The main input requirements of the REEDM program are meteorological data in the form of rawinsonde measurements and rocket vehicle parameters. Rawinsonde profiles of wind speed and direction, temperature and dew point, barometric pressure, relative humidity, and air density are required up to approximately 3,000 m (10,000 ft). Meteorological tower and doppler acoustic sounder measurements of wind direction and elevation angle standard deviations may optionally be used to specify atmospheric turbulence. Other meteorological parameters required by the model include the cloud cover, cloud ceiling height, and mixing depth. Rocket vehicle parameters (source inputs) required by REEDM depend on the vehicle and launch scenario.

Default rocket vehicle parameters are provided in a data base file for the space shuttle, Titan II, Titan 34D, Titan IV, Delta 2914, Delta 3914, and Minuteman II. In general, the required vehicle parameters for SRB's are the solid fuel load, the solid fuel burn rate, the heat released per unitmass of the solid fuel, and the pollutant (hydrogen chloride, aluminum oxide, etc.) emissions per unit mass of the solid fuel. Similarly, the required vehicle parameters for hypergolic rocket engines are the total liquid fuel and oxidizer loads, the fuel and oxidizer flow rates, and the time after SRB ignition of the ignition of the liquid engine. Rocket vehicle parameters required for both solid motors and liquid hypergolic engines include the coefficients a, b, and c of the equation

$$t = ah^{b} + c \quad , \qquad (11.1)$$

where t is time and h is vehicle height above ground level. Finally, the REEDM program has an option to use a mesoscale wind field model to account for the effects of complex terrain on the low-level circulation (Fig. 11-1). The use of this feature required terrain elevations for a grid system surrounding the launch site.

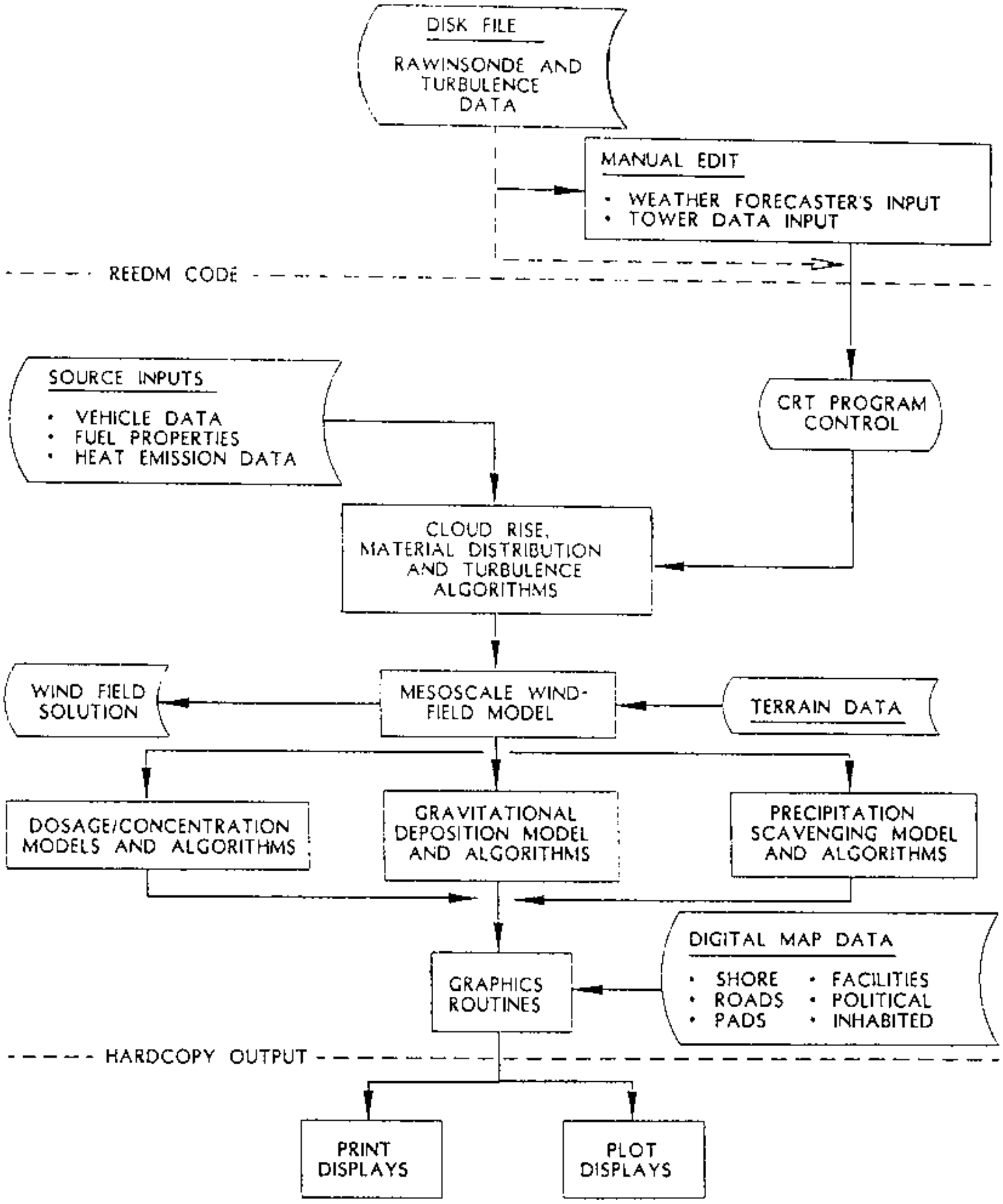

FIGURE 11-1. Schematic Diagram Illustrating the Major Components of the REEDM Computer Program.

Table 11-6. Summary of computer models available for hazard assessment.

Model	Type	Applicability	Meteorological Inputs	Source Inputs	Output
REEDM	Gaussian diffusion model coupled to a wind field model.	Static firings, normal launches, conflagrations, and deflagrations.	Rawinsonde profiles, cloud cover, ceiling height, and mixing depth. If available, tower or Doppler acoustic sounder wind direction and elevation angle measurements may be used as turbulence inputs.	Fuel load, fuel burn rate, fuel heat content, and pollutant emissions per unit weight of fuel burned. Coefficients of vehicle time-height curve also required for normal launches and deflagarations.	Peak concentration and dosage; time-mean concentration; cloud arrival and departure times; gravitational deposition and precipitation washout (maximum deposition or minimum pH). Plume rise, cloud position, and turbulence parameters may also be output. Graphics output is available.
HARM	Gaussian diffusion model.	Hypergolic expolsions above ground or in silos.	Rawinsonde profiles, cloud cover, ceiling height, and mixing depth.	Accident type and quantities of fuel and oxidizer released.	Peak concentration and dosage; time-mean concentration; cloud arrival and departure times; and precipitation washout. Graphics output is available.

Table 11-6. Summary of computer models available for hazard assessment (continued).

Model	Type	Applicability	Meteorological Inputs	Source Inputs	Output
AFTOX	Gaussian diffusion model.	Instantaneous and continuous liquid and gas releases. Includes buoyant rise for stack plumes and evaporation for spills.	Surface roughness length, cloud cover, ceiling height, wind speed and direction, air temperature, and mixing depth. Standard deviation of wind direction is optional turbulence input.	Type of release and quantity, molecular weight, and vapor pressure of chemical released. Contains data base of properties for 76 chemicals. Additional inputs required for stack releases.	Concentration at user-specified times. Graphics output is available, including 90 percent confidence limits on hazard distances.
D2PC	Gaussian diffusion model.	Instantaneous, quasi-continuous and continuous liquid and gas releases. Includes evaporation for spills. Designed primarily for application to chemical warfare agents.	Cloud cover, ceiling height, wind speed and direction, air temperature, barometric pressure, and mixing depth. Pasquill stability category can be entered to replace category determined from cloud cover/ceiling height and wind speed.	Essentially the same as AFTOX.	Peak concentration and dosage. Hazard distances to 1-percent lethality, no deaths, and no effects for chemical munitions.
OB/DG	Empirical diffusion model equation.	Continuous release at the surface (usually an evaporative spill).	Wind direction, wind direction standard deviation, and temperature difference between 56 and 6 ft.	Evaporation rate.	Downwind distance to specified concentration. Some versions predict 95-percent confidence limit on hazard distance.

Table 11-6. Summary of computer models available for hazard assessment (continued).

Model	Type	Applicability	Meteorological Inputs	Source Inputs	Output
BLAST	Acoustic.	Sonic boom propaga-tion.	Rawinsonde profiles.	Vehicle flight profile.	Focus overpressures. Some versions estimate window damage.
BOOM	Acoustic.	Maximum overpressure for a surface noise source.	Rawinsonde profiles.	TNT equivalent of noise source.	Instantaneous overpressure.

Table 11-7. Summary of computer resources required by hazard assessment models.

Model	Computer Language	Specific Computers	Program Size	Comments
REEDM	FORTRAN 77	Mainframe IBM compatible PC-AT	Source code: 1.3 Mbytes Executable code: 1.33 Mbytes	Program can be segmented to reduce memory requirements.
HARM	FORTRAN 77	Mainframe	750,000 bytes	
AFTOX	BASIC	IBM compatible PC Zenith-100 Zenith-248		Two versions, one for Zenith-100 and one for Zenith-248.
D2PC	FORTRAN 77	Mainframe or PC	<200,000 bytes	
OB/DG	Many different versions exist	Scientific calculator		Many computerized versions exist for different applications.
BLAST	FORTRAN 77	Mainframe		
BOOM	BASIC	Microcomputer Radio Shack TRS-80 PC-2		

The REEDM program output options include tables of peak concentrations, total dosages, cloud arrival and departure times, and time-mean concentrations at user-specified downwind distances; tables of maximum ground-level deposition at user-specified downwind distances; and tables of precipitation deposition expressed as either maximum deposition or minimum surface water pH at user-specified downwind distances. The program produces a summary or very detailed print output, depending on the mode of operation. The more detailed print output includes intermediate calculations such as plume rise, cloud position, and turbulence parameters. Graphics output options consist of plots of vertical profiles of the meteorological data; plots of centerline peak or time-average concentration, dosage, or deposition versus downwind distance; and isopleth (contour) plots of peak or time-mean concentration, dosage, and deposition. Examples of REEDM plots of centerline peak concentration and peak concentration isopleths are shown in figures 11-2 and 11-3, respectively.

The REEDM version 7 computer program is written in FORTRAN 77 and is designed for use on CDC CYBER 700, UNIVAC 1100, HP9000/800, and VAX 780 or 8000 series computers. The source program is 1.3 megabytes in length and the executable program requires approximately 1.33 megabytes of memory. The graphics output requires either a Calcomp 36-in drum plotter or a Tektronix 41xx terminal. An IBM PC-AT compatible adaptation of the REEDM version 7 code has recently been completed.

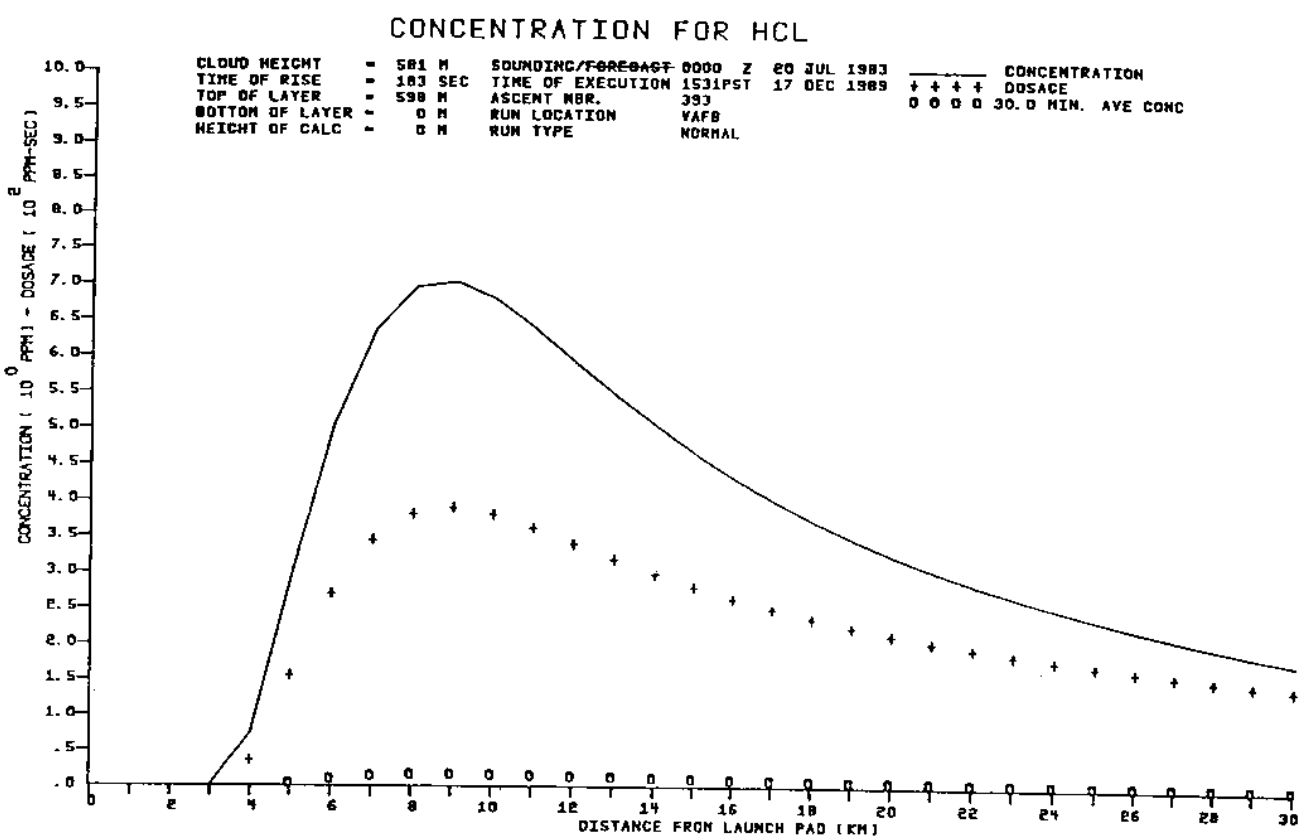

FIGURE 11-2. Example REEDM Plot of Centerline Peak HCl Concentration Versus Downwind Distance for a Space Shuttle Launch.

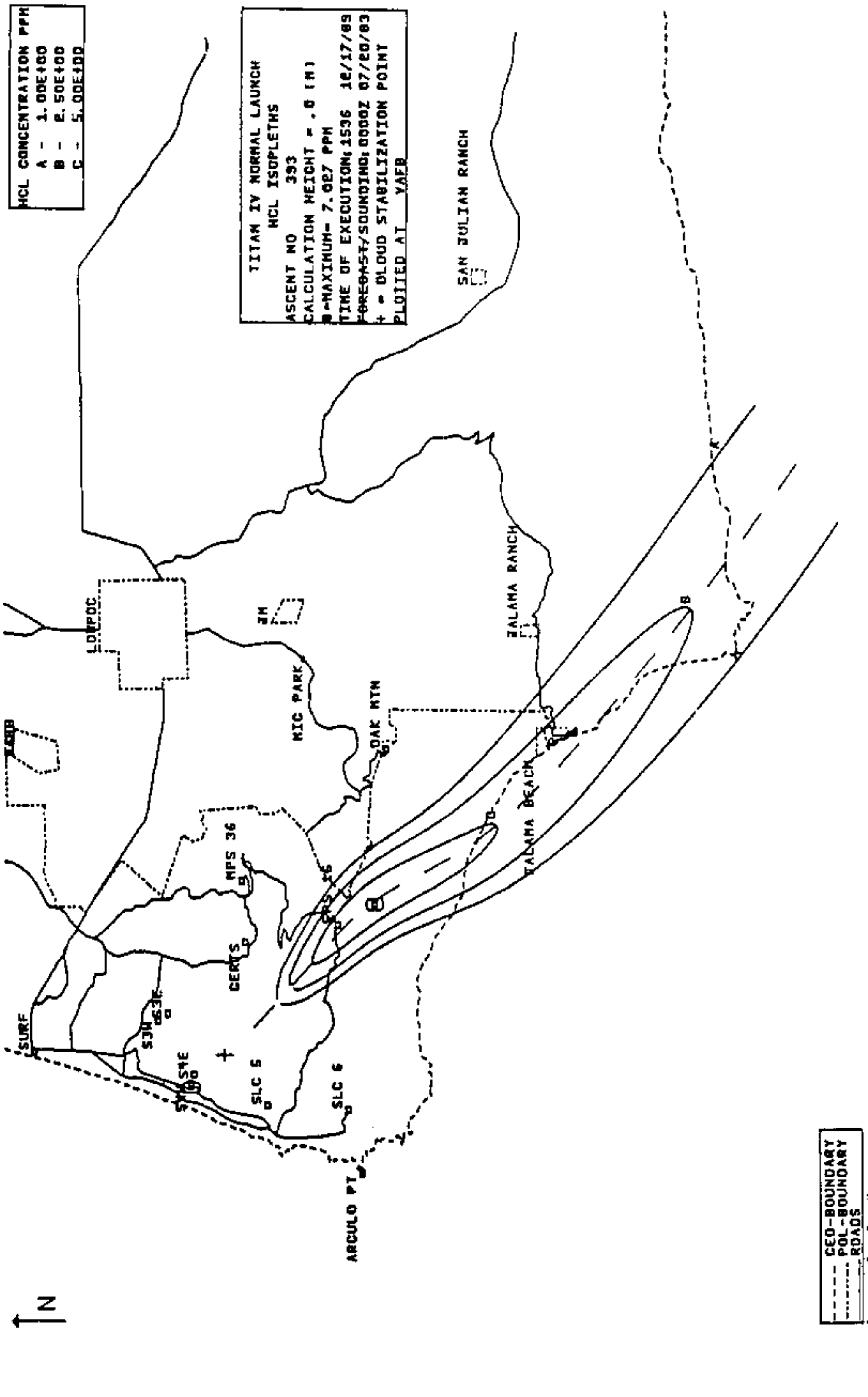

Figure 11-3. Example REEDM plot of peak HCl concentration in parts per million for a space shuttle launch.

11.8.3 HARM. The hypergolic accidental release model (HARM) (ref. 11.17) combines source characterization algorithms for hypergolic reactions (refs. 11.18 and 11.19) with the REEDM cloud rise and dispersion algorithms to predict the transport and dispersion of toxic clouds produced by hypergolic reactions. The four hypergolic accident scenarios that can be considered by the model are: (1) above ground, (2) in-silo with the silo door closed, (3) in-silo with the silo door open, and (4) ejected second stage detonation resulting from an in-silo explosion. The HARM computer program calculates peak concentration, dosage, time-mean concentration, and deposition due to precipitation scavenging (washout) at points downwind from the accident site. If the precipitation scavenging option is selected, the user may direct the program to predict either the maximum possible washout for the user-specified rainfall rate or the washout expected for the user-specified rainfall rate and precipitation start and end times.

The HARM computer program has operational, research, and production run modes. The operational mode, which is designed for real-time use during emergencies or accidents, automatically selects many of the required input parameters. The research mode allows the user greater freedom in specifying inputs and provides more detailed output, while the production mode is used to process multiple cases, usually in a batch environment.

The HARM program's meteorological inputs consist of rawinsonde profiles, the depth of the surface mixing layer, and the base and top of an elevated layer within which concentration or dosage predictions are desired. Other inputs include the cloud cover and ceiling height, the accident type, and the quantities of fuel and oxidizer released.

The HARM program's printed output consists of tables listing the upper-air sounding; stabilized cloud parameters; peak concentration, time-mean concentration, and dosage values along with range, bearing, and cloud arrival and departure times; and precipitation washout along with range and bearing. Graphics output options consist of: (1) vertical profiles of meteorological parameters plus the cloud shape at stabilization; (2) profiles of centerline concentration, dosage, and time-mean concentration or washout versus downwind distance for user-specified toxic chemicals; and (3) isopleths of concentration, dosage, and time-mean concentration or washout. The isopleths can be plotted on a standard map of the area.

The HARM computer code is written in FORTRAN 77 and requires no special computer facilities. Hardcopy printing and plotting facilities are helpful, but not required. Approximately 750,000 bytes of memory are used by the HARM code.

11.8.4 AFTOX. The U.S. Air Force toxic chemical dispersion model (ref. 11.20) is an interactive computer program designed to predict toxic chemical concentrations and dosages downwind of an accidental release. The program can also predict the dispersion of a buoyant stack plume. AFTOX is based on SPILLS, a model developed by the Shell Oil Company (ref. 11.21).

The AFTOX model requires chemical, source, and meteorological inputs. The AFTOX program contains a data file of the properties of 76 toxic chemicals. If the chemical to be modeled is not in this file, the model will request the chemical's molecular weight and vapor pressure. The molecular weight is used to convert concentrations to units of parts per million, while the vapor pressure is used in the evaporation calculations. If the molecular weight is not known, concentrations must be output in units of milligrams per cubic meter. If the vapor pressure is not known, AFTOX makes the worst-case assumption that the evaporation rate equals the spill rate. The program allows the user to update or modify its chemical data file. The

AFTOX model's source inputs consist of the type of release (continuous or instantaneous, liquid and/or gas) and parameters that are dependent on the type of release. For a stack, these inputs include the emission rate, volumetric flow rate, and exit temperature. For a chemical spill, these inputs include the spill rate, total time of release, height of release, area of spill, and pool temperature. The AFTOX model's meteorological inputs consist of the air temperature, wind speed and direction, standard deviation of wind direction (optional), sky cover and cloud category (low, middle, or high), ground condition, and mixing layer height.

Three output options are available with the AFTOX program: (1) a plot of concentration isopleths for up to three user-specified contour values, (2) the concentration at a user-specified location and time, and (3) the maximum concentration at a user-specified height and time after the spill. If the plot option is selected, the isopleth plot includes a hazard sector that represents the area expected to contain the minimum contour value approximately 90 percent of the time. This feature accounts for the fact that the concentration predicted by a diffusion model at a given downwind distance is the mean value that would be expected at that distance if the same release were made a number of times under similar meteorological conditions. Thus, hazard distances longer than indicated by the concentration isopleth can be expected about 50 percent of the time. All AFTOX output is directed to the user's terminal.

There are two versions of AFTOX, both written in the BASIC language. Version 1 was designed specifically for use on the Zenith-100 microcomputer and version 2 was designed for the Zenith-248 microcomputer. Both versions are IBM compatible, with version 2 having an enhanced color graphics capability. Hardcopy graphics and text output can be sent to a printer if available. Execution times for AFTOX can become large for cases with long downwind hazard distances. These times can be reduced by approximately a factor of 10 if a BASIC compiler is used to produce a directly executable binary copy of AFTOX.

11.8.5 D2PC. The U.S. Army chemical hazard prediction model D2PC (ref. 11.22) calculates peak concentrations and dosages and downwind hazard distances for continuous, instantaneous, or variable releases of toxic chemicals. The D2PC program is a revised version of the D2 program (Ref. 11.23) that includes a more user-friendly input environment and a vapor depletion option that considers losses by deposition/ground absorption and/or atmospheric chemical reactions. The D2PC program is primarily designed to provide the U.S. Army's chemical weapons storage facilities with a tool to estimate downwind hazard distances for accidental releases of chemical agents. Although the release scenarios built into D2PC are for chemical weapons, the program can estimate downwind concentrations and dosages for releases of most toxic materials by entering user-defined input parameters.

The D2PC program contains a rather broad data base that includes: (1) the location, average pressure, and seasonal average mixing layer heights of 11 U.S. Army chemical storage sites; (2) source parameters for 10 different chemical munitions; and (3) the physical constants, such as molecular weight, for 17 different toxic chemicals (including UDMH and hydrazine). If the accident/incident site, type of munition, or toxic chemical of interest is not in the D2PC data base, the user must provide the required information. Additional input parameters include the amount of chemical released, the type of release (explosion, evaporation, flash fire, etc.), the surface type and puddle dimensions for a spill, and the meteorological conditions (atmospheric stability, wind speed, ambient air temperature, barometric pressure, and mixing height). The user can select a Pasquill stability category or have the program estimate the stability category from the wind speed, cloud cover and height, date and time, and location. If the model is used in a wooded area, stability is not required because the dispersion rate is assumed to be a function only of the wind speed outside the woods.

The D2PC program provides print output only, and the user determines how descriptive this output will be. The output consists of a listing of the input parameters and the results of the concentration or dosage calculations. The default output, which is specifically designed for application to chemical agents, provides the approximate downwind hazard distances for 1-percent lethality, no deaths, and no effects. The user can also choose to have downwind distances calculated for specified dosage or concentration values.

The D2PC program is written in FORTRAN 77 for use on IBM-compatible personal computers. A hardcopy output device is useful but not necessary. The program requires less than 200,000 bytes of memory to execute. The program has also been run on mainframe computer systems. Because D2PC is written in FORTRAN 77, it is an alternative to the BASIC-coded AFTOX spill model.

11.8.6 Ocean Breeze/Dry Gulch (OB/DG). The Ocean Breeze and Dry Gulch (OB/DG) diffusion model (ref. 11.24) is an empirical equation that predicts centerline concentration as a function of downwind distance for a ground-level release. The OB/DG equation was developed by the U.S. Air Force to consider the downwind hazards of accidental spills of propellants from the Titan II missile at Cape Canaveral, Florida and Vandenberg Air Force Base, California. The model is based on three field experiments conducted by the Air Force Cambridge Research Laboratories. The first, Project Prairie Grass (refs. 11.25–11.27), was conducted near O'Neill, Nebraska. The other two diffusion experiments took place at Cape Canaveral and Vandenberg Air Force Base and were named Ocean Breeze (ref. 11.28) and Dry Gulch (ref. 11.29), respectively. The composite data set from the Prairie Grass, Ocean Breeze, and Dry Gulch experiments was divided into two, with the first half of the data used to derive the OB/DG model equation and the second half used to test it. The regression fit to the first half of the data yielded

$$Cp/Q = (0.00211)\, X^{-1.96}\, \sigma_\theta^{-0.506}\, (\Delta T + 10)^{4.33}\,, \qquad (11.2)$$

where

Cp = peak (centerline) concentration (g/m^3) at downwind distance X(m)

Q = release rate (g/s)

σ_θ = standard deviation of wind direction (degree)

ΔT= temperature difference (°F) between 56 and 6 ft.

Wind speed was initially considered in deriving the OB/DG equation, but was deleted because it did not significantly improve prediction accuracy. Because of the difficulty in obtaining σ_θ from the traces produced by the analog recorders in use at Titan II sites at that time, a second regression equation was derived in which ΔT is the only meteorological predictor.

The second half of the composite data set from the Prairie Grass, Ocean Breeze, and Dry Gulch experiments was used to evaluate the OB/DG equation and determine confidence limits. The peak concentrations predicted by the equation agreed to within a factor of 2 of the observed concentrations for 72 percent of the cases and to within a factor of 4 for 97 percent of the cases. After solving the OB/DG equation for the downwind distance to a hazard concentration, the Air Force normally multiplies this distance by 1.63 to obtain a 95-percent confidence that concentrations above the hazard level will not occur at longer downwind distances.

The OB/DG model is limited by its empirical basis. For example, it generally predicts shorter hazard distances than other diffusion models at night with stable meteorological conditions because it is principally based on day-time trials. Also, it is not applicable to instantaneous releases or to large buoyant clouds or plumes. Because the OB/DG model considers peak concentrations only, it cannot provide information on ground-level concentration patterns.

The advantage of the OB/DG model is that it requires minimal meteorological inputs and computer resources. Consequently, it has served for decades as a simple way of estimating hazard distances downwind of spills of toxic propellants. Over the years, the OB/DG equation has been implemented in forms ranging from nomograms to computer programs. Many variations and modifications such as changes in units of input parameters have been made for specific applications. If an existing OB/DG computer program is used, the exact model formulation should therefore be determined.

11.8.7 BLAST. The BLAST model is designed to predict the propagation of sonic booms. Based on the original work by Plotkin (ref. 11.30), BLAST was developed for use by the U.S. Air Force at the Eastern and Western Test Ranges. The model uses rawinsonde profiles of pressure, temperature, and winds as meteorological inputs and the flight profile as source inputs. Some versions of BLAST go beyond the prediction of sonic boom focus overpressures and combine population densities with predicted overpressures to estimate window damage. Worst-case analyses can be performed by allowing BLAST to modify the rawinsonde profiles in order to maximize the overpressures predicted at the surface. The interpretation of the BLAST computer program's output is rather difficult and requires experience.

11.8.8 BOOM. The blast operational overpressure model (BOOM) (ref. 11.31) was developed by the U.S. Air Force to predict the far-field acoustic overpressures produced by explosions at the surface. Rather than use computer intensive ray tracing techniques, BOOM uses a simple, semi-empirical equation to predict the instantaneous overpressure. This equation is based on the maximum value of $\Delta v/\Delta z$, where Δv is the difference in sound between the surface and height Δz above the surface. The BOOM computer program determines the vertical profile of the speed of sound from rawinsonde profiles of pressure, temperature, and winds. The model's empirical coefficients are based on data from two sets of surface detonations. Although BOOM is specifically designed for application to explosions at the surface, it can be applied to any surface sound source that can be defined in terms of the TNT equivalent explosive weight. The BOOM computer code is written in BASIC and is specifically designed for use on a Radio Shack TRS-80 PC-2 portable microcomputer.

An elaborate, site-specific, sound propagation model (ref. 11.32) called “Noise Assessment and Prediction System” (NAPS), is now in place at Aberdeen Proving Ground, MD. However, it is currently being made transportable for use at other ranges. It is an automated program/system which includes ray-tracing and sound-level contouring, etc.

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